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# ATABS - AN EASY TO USE, COMPUTER PROGRAM FEATURING COMPLETE PROCESSING OF ATOMIC ABSORPTION DATA AND COMPREHENSIVE DISSPLA*** GENERATED GRAPHICAL OUTPUT

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# ATABS - AN EASY TO USE COMPUTER PROGRAM FEATURING COMPLETE PROCESSING OF ATOMIC ABSORPTION DATA AND COMPREHENSIVE DISSPLA*** GENERATED OUTPUT

by

K. Bartels* and P.L. Bédard**

## SUMMARY

ATABS is a computer program which enables "one-pass" computer computation and plotting of atomic absorption analysis data. ATABS calculates results for both the matrix calibration curve and measured samples, and specifically features graphical output on the Computer Science Centre Calcomp 1051 drum plotter using the recently-acquired DISSPLA plotting software. ATABS thereby eliminates all hand calculations and manual plotting of data. The job deck structure has been designed to facilitate usage even by those chemists and technicians with little or no knowledge of computing so that they can successfully process atomic absorption data.

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***DISSPLA is a proprietary product of ISSCO, San Diego, California, U.S.A.

# ATABS: UN PROGRAMME INFORMATIQUE D'UTILISATION SIMPLE PERMETTANT LE TRAITEMENT COMPLET DES DONNÉES D'ABSORPTION ATOMIQUE ET UNE SORTIE COMPLÈTE GÉNÉRÉE PAR DISSPLA***

par

K. Bartels* et P.L. Bédard**

## RÉSUMÉ

ATABS est un programme informatique permettant d'effectuer "en une passage" sur ordinateur le calcul et le traçage des données de l'analyse par absorption atomique. ATABS calcule des valeurs pour la courbe d'étalonnage de matrice et pour des échantillons mesurés, et permet une sortie graphique sur le traceur à tambour Calcomp 1051 du Centre d'informatique, à l'aide du logiciel de traçage DISSPLA acquis récemment. ATABS élimine donc toutes les opérations manuelles de calcul et de traçage. Le paquet de cartes est structuré de façon à permettre l'utilisation du programme même par des chimistes et des techniciens connaissant peu ou pas du tout l'informatique, afin qu'ils puissent traiter sans difficulté les données d'absorption atomique.

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***DISSPLA est une produit breveté de l'ISSCO, San Diego (California), É.-U.

## INTRODUCTION

In view of the large number of samples which are daily analysed at CANMET by atomic absorption spectrophotometry and with the recently acquired DISSPLA plotting software providing greatly improved graphical output, it was felt that a "one-pass" calculating/plotting program would prove a great time-saver for laboratory staff responsible for AA analyses. This report describes procedures by which job execution may be achieved and provides examples of job deck set-ups for submission to the CYBER/NOS-BE system. Data may be processed either as a deck of punched cards through a card reader or as a local file batched from an on-line terminal. The program is stored as a relocatable binary on the CSC permanent files. The source code is not described in detail, but a general description of the execution procedure of ATABS is provided.

In designing ATABS it was assumed that a typical "manual" AA analysis consists of determining calibration points in the required matrix over a range of concentrations which encompass the minimum and maximum of the expected concentrations of the element being analysed (e.g., Pb). It was further assumed that the percent absorption of the calibration matrix is set to zero at 0 µg/g concentration of the element. Once the calibration data have been measured, it is then the usual procedure to construct manually a calibration curve from which the µg/g concentrations of the unknowns are read once their absorbances are determined. This "manual" procedure has, in some cases, been partially augmented by the use of hand or desk-top calculators and/or desk-top calculator/plotters. Some computer generated least-squares fitting routines have been used to determine a "best-fit" calibration curve and its respective equation, but to the knowledge of the authors, a "one-pass" computation/plotting program does not presently exist within CANMET. The program ATABS has, therefore, been designed to eliminate all "manual" manipulation of data, save that of entering the input data into the appropriate file for execution.

## PROGRAM DESCRIPTION

### 1. Program Execution Steps

(a) ATABS reads the following from the input file:
- sample #, sample description and plot parameters (first five lines)
- calibration data consisting of known concentrations (µg/g) and their respective absorbances
- absorbance data for samples of unknown concentrations

(b) The program sets up the plot using the plot parameters and the maxima and minima of the concentration and absorbance values which it calculates from the calibration data. Concentration is plotted on the abscissa (x-axis) and absorbance is plotted on the ordinate (y-axis).

(c) ATABS calculates the parameters for the second-order polynomial

$$\mu g/g = a_1(\text{absorbance}) + a_2(\text{absorbance})^2$$

which best fits the calibration data. The best fit is achieved by standard least squares procedures. A fit to this type of polynomial ($y = a_1x + a_2x^2$), lacks the constant term $a_o$ (the y-intercept) and thereby forces the fit through the origin (0,0).
Finally ATABS calculates µg/g concentrations for the corresponding absorbances of the unknowns, using the above equation and the calculated values of $a_1$ and $a_2$.

### 2. Output provided by ATABS

As output, ATABS provides the following:
- a listing (Fig. 1) of the sample descriptors (i.e., sample # and sample type), the calibration data, the regression calibration equation and a limited residual analysis to enable users to determine calibration points which may not have been accurately measured.
- a listing of the observed absorbance and calculated µg/g concentrations of the unknowns.
- a DISSPLA generated CALCOMP plot (Fig. 3) which includes:

(a) the calibration data (open octagons)

(b) the fitted equation (solid line)

(c) the measured absorbances and calculated concentrations of the unknown samples (+'s).

(d) graph title, x- and y-axis titles as determined by the plot parameters

(e) fully numbered x- and y- axes whose ranges incorporate the full extent of the calibration data.

(f) appropriate labels indicating user name and plot delivery address as designated in the control card deck.

## 3. Error Returns

Appropriate messages will be printed on the line printer and the program will abort when:

- more than 20 calibration points are entered.
- more than 50 unknowns are entered.

For concentrations of unknowns which fall outside the range of the calibration curve, DISSPLA provides the appropriate error messages.

# JOB DECK STRUCTURE, CONTROL CARD DECK AND DATA DECK SET-UP

## 1. Job Deck Structure

The standard job deck structure required by the CYBER/NOS-BE computer system is given in Fig. 4. It should be noted that "End of Records" are multipunch 7/8/9 cards for a punched-card deck and *EOR statements for files created in "EDITOR" or "TXTEDIT". Similarly, "End of Information" are multipunch 6/7/8/9 cards and *EOF statements in punched-card decks and batch files, respectively. A typical punched-card deck processed from a card reader is shown in Fig. 5 and a typical batch file created in "EDITOR" is shown in Fig. 6. The two decks differ only in their "End of Records" and "End of Information".

## 2. Control Card Deck

With respect to Figures 5 and 6, the control card deck consists of cards 1 to 5. Its end is signified by the first "End of Record", card 6. In place of "BARTELS", each user would insert (in Card 1 and 4) his or her own name and appropriate delivery stop # and on card 2 his or her own ACCOUNT #. In the case of the example of Figures 5 and 6, the plot was labelled Bartels, Stop 10 (Fig. 3) and therefore was delivered to Room 126 at 555 Booth Street.

Each complete plot requires about 11 inches of paper in the x-direction. The value of XSIZE = 100 has been included as a safety measure and therefore up to 8 data sets may be plotted before DISSPLA would abort the job. Each user may, however, increase this value as required.

## 3. Data Deck Set-up

With respect to Figures 5 and 6:

Card 7 (data card no. 1):

Columns 1 to 9 incl: up to ten alphanumeric characters may be inserted here for use as sample #.

Columns 10 to 19 incl: must be blank

Columns 20 to 80 incl: up to sixty alphanumeric characters may be inserted here to describe the sample type.

Card 8 (data card no. 2):

Columns 1 to 80 incl: this is the title of the plot (Fig. 3). It must end with a $ sign. The $ will not be plotted; it is required so that DISSPLA will know the number of characters in the title and thus be able to centre it over the plot. The maximum number of characters allowed as a plot title, including the $ sign, is thirty. However, to enhance the plot, provision has been made for capitalization of lettering. Thus any letters which are to appear as capitals (i.e., upper case) should be enclosed in left and right

fleches (<>). These two and the plus (+) have been reserved as DISSPLA instruction characters**. Although the actual title plotted may not exceed 30 characters, up to 80 characters are allowed on the input data cards for titles to enable the inclusion of DISSPLA instruction characters. Under these rules, the following would apply:

(a) the input string: PBCL2$ results in a plot of pbcl2.

(b) and the input string: <P>B<C>L2$ results in a plot of PbCl2.

Since the $ sign is required by DISSPLA to test for the end of the input string, it must always appear in the lower case: (i.e., it must never follow a left fleche (<)).

Thus the string

<P>b<C>12 BY<A A$> would abort,

whereas <P>b<C>12 BY<A A>$ would result in the plot of PbCl2 by A A.

Card 9 - data card no 3: the x-axis title (same DISSPLA rules as for the plot title apply).

Card 10 - data card no 4: the y-axis title (same DISSPLA rules as for the plot title apply).

Card 11 - data card no 5: the legend title - this would most suitably be the sample number. Only 20 characters may be plotted as a legend title (same DISSPLA rules as for the plot title apply).

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* < = upper case R or numeric multipunch 12-2-8 on 026 card punch
  > = upper case G or numeric multipunch 11-7-8 on 026 card punch

** The plus (+) is the instruction character initiating the lower case "Greek" alphabet enabling the writing of the lower case mu (μ) on the x-axis title of Fig. 3. For those programmers familar with DISSPLA instruction strings, the shriek (!) has also been reserved as the character signalling the instruction alphabet (i.e., CALL MX6ALF ("INSTR", "!"), so that the input data card <P>B<C>L!LH.8>2!LXHX>$ would result in the plotting of $PbCl_2$ - namely upper case P and C as well as a subscripted 2.

Cards 12 to 16 incl: the calibration data entered as pairs of data per line, where

μg/g abs

is equivalent to x- and y-axis data, respectively. Entry is in the form of free-field data in which data pairs are separated by either a blank space or a comma. Thus,

5.0 0.185

5.0,0.185 are both correct.

Superfluous decimal points are not required. For example, 5.0, 5. or 5 all give the same result.

The end of calibration data is signalled by the appropriate "End of Record" (line 17). A maximum of 20 calibration points is allowed.

Cards 18 to 24: Measured absorbances of unknowns - one absorbance value per line. The appropriate "End of Records" signals the end of the absorbance data for the unknown.

More than one subsequent complete input data set may be plotted on additional graphs. These additional data sets are simply entered between lines 25 and 26 and should be composed of a complete input data file as depicted by lines 7 to 25. Thus the following configuration would plot three separate AA plots.

CONTROL CARD DECK
7/8/9
Data Deck 1 (line 7 to 24 incl)
7/8/9
Data Deck 2 (similar to lines 7 to 24 incl)
7/8/9
Data Deck 3 (similar to lines 7 to 24)
7/8/9
6/7/8/9

As mentioned before, XSIZE = 100 limits multiplots to only 8 data sets but users are free to increase this limit.

## SUMMARY

ATABS has been written to enable "one-pass" calculation and plotting by computer of a standard set of atomic absorption data consisting of calibration data and measured absorbances of a series of unknowns. Standard least-squares minimization fitting of the calibration data, calculation of the concentration of the unknowns from the fitted calibration data, a comprehensive plot and full output listings are all provided by ATABS. It is necessary for the user only to enter the required data in a free-field format. Plot enhancement due to the reservation of DISSPLA characters for DISSPLA instruction strings is possible. ATABS eliminates all hand calculation and manual plotting, and has been found to save time when processing AA data. More important, it provides a more accurate indication of the unknown concentrations than is possible with manually determined calibration graphs.

## ACKNOWLEDGEMENT

The authors sincerely thank Bill Bowman of MSL, CANMET, for the use of his regression subroutine and his valuable comments during the development of the program.

* * * ATOMIC ABSORPTION CALIBRATION CURVE * * *

SAMPLE #: PBCL2- 002 SAMPLE TYPE: PBCL2 IN 0.1 N HCL

CALIBRATION SUMMARY

PARAMETERS FOR PLOT 1

PLOT TITLE : <P>B<C>L2 BY <A A>S
X-AXIS TITLE: <P>B<C>L2 (*M>G/GIS
LENGTH IN INCHES = 7.0 RANGE = 0.00 TO 30.00
Y-AXIS TITLE: <A>BSORBANCES
LENGTH IN INCHES = 9.0 RANGE = 0.00 TO .88
LEGEND TITLE: <P>B<C>L2- 002S

CALIBRATION DATA

| NO. | MICCAL | ABSCAL |
|---|---|---|
| 1 | 0.00 | 0.000 |
| 2 | 5.00 | .185 |
| 3 | 10.00 | .369 |
| 4 | 20.00 | .649 |
| 5 | 30.00 | .875 |

| TERM NO. | COEFFICIENT |
|---|---|
| 1 | 2.24487E+01 |
| 2 | 1.33793E+01 |

| OBS. NO. | MICCAL | ABSCAL | PRED. MICCAL | RESIDUAL | % RESIDUAL |
|---|---|---|---|---|---|
| 1 | 0.00 | .000 | .00 | -.00 | 0.00 |
| 2 | 5.00 | .185 | 4.61 | .39 | 8.44 |
| 3 | 10.00 | .369 | 10.11 | -.11 | 1.04 |
| 4 | 20.00 | .649 | 20.20 | -.20 | 1.01 |
| 5 | 30.00 | .875 | 29.89 | .11 | .38 |

THE REGRESSION EQUATION FOR THE CALIBRATION DATA IN TERMS OF THE UNKNOWN CONCENTRATION (MICRO G/G) IS :

MICRO G/G = 2.244869E+01*ABSNCE + 1.337929E+01*ABSNCE**2



Fig. 1 - Page 1 of output listing which includes sample descriptors, plot parameters and calibration data.

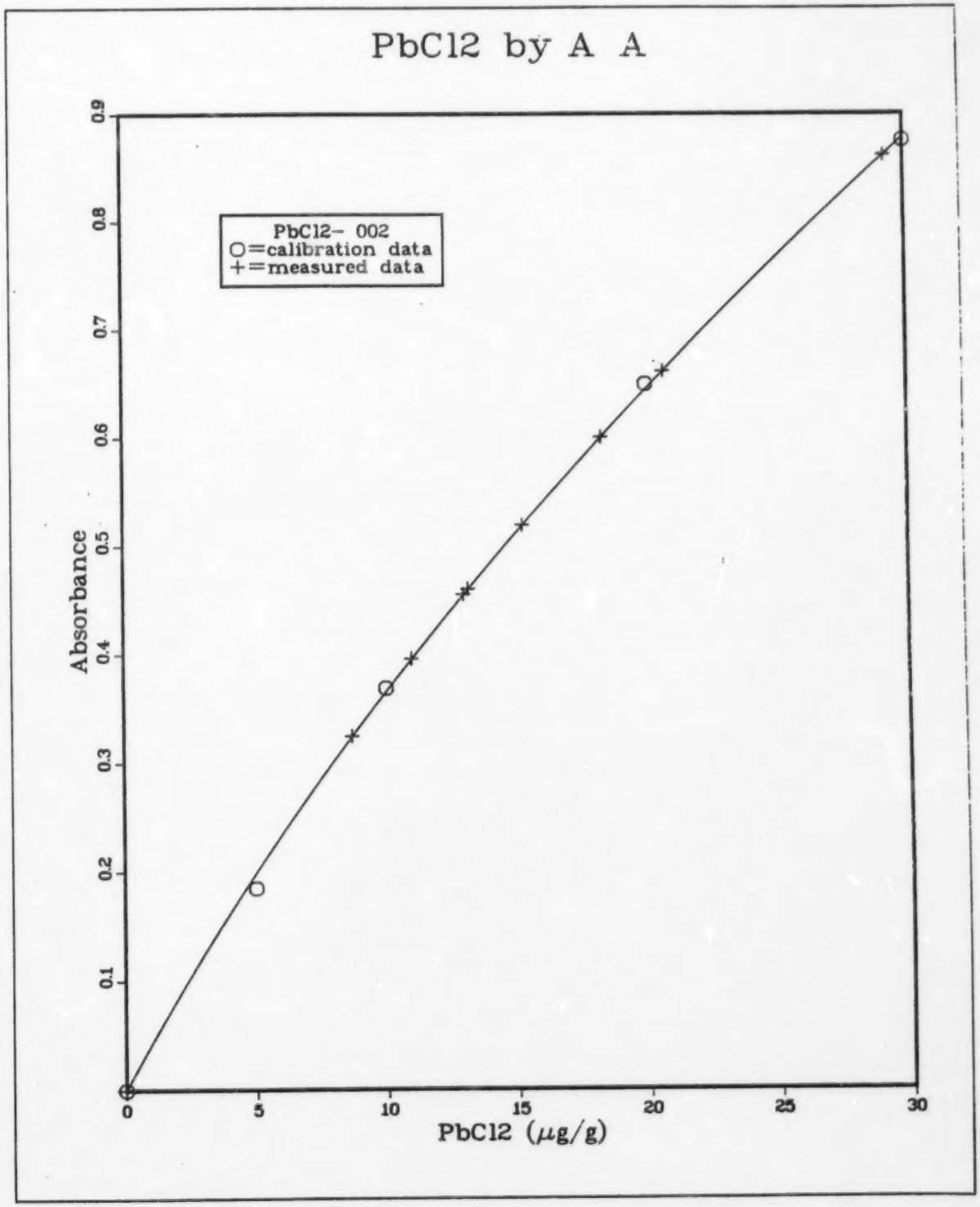
* * * ATOMIC ABSORPTION DATA FOR MEASURED SAMPLES OF UNKNOWN CONCENTRATION * * *

SAMPLE #: PBCL2- 002 SAMPLE TYPE: PBCL2 IN 0.1 N HCL

| NO. | (ABSNCE) | (MICRO G/G) |
|---|---|---|
| 1 | .396 | 10.988 |
| 2 | .600 | 18.286 |
| 3 | .455 | 12.984 |
| 4 | .661 | 20.684 |
| 5 | .460 | 13.157 |
| 6 | .519 | 15.255 |
| 7 | .325 | 8.709 |
| 8 | .861 | 29.247 |



Fig. 2 - Page 2 of output listing which includes the observed absorbance of unknowns and calculated concentrations.




BARTELS STOP 10
C278050 C27805D19 19/02/82 12.37.11. TYPE 2

Fig. 3 - Example of DISSPLA generated CALCOMP plot of AA data.

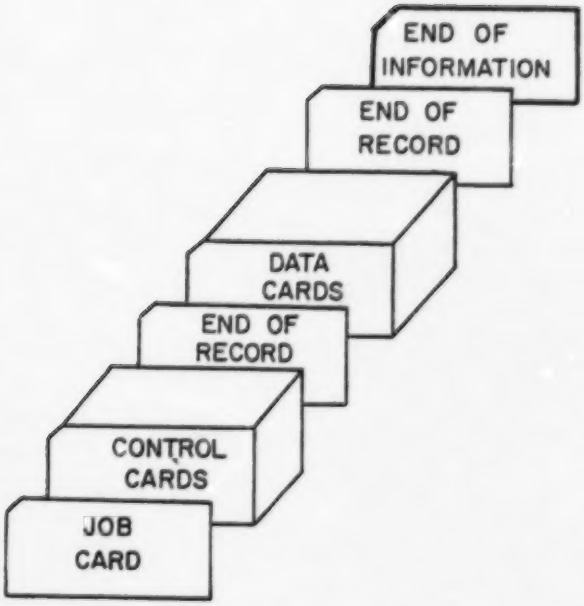



Fig. 4 - Job Deck Structure

```
C2780,CM120000,P2. BARTELS                                    CARD 1
ACCOUNT,*****. ATABS                                             2
ATTACH,ATB,ATABSBIN,ID=JED,CY=10,MR=1.                           3
BEGIN,DISSPLA,,CAL1051,NAME=$BARTELS STOP 10$,                   4
TYPE=2,P1=NIB,S1=3,PAPER=11,XSIZE=100,B=ATB.                     5
7/8/9                                                            6
PBCL2- 002          PBCL2 IN 0.1 N HCL                           7
<P>B<C>L2 BY <A A>$                                              8
<P>B<C>L2 (+M>G/G)$                                              9
<A>BSORBANCE$                                                   10
<P>B<C>L2- 002$                                                 11
0.0 0.0                                                         12
5.0 0.185                                                       13
10.0 0.369                                                      14
20.0 0.649                                                      15
30.0 0.875                                                      16
7/8/9                                                           17
0.396                                                           18
0.600                                                           19
0.455                                                           20
0.661                                                           21
0.460                                                           22
0.519                                                           23
0.325                                                           24
0.861                                                           25
7/8/9                                                           26
6/7/8/9                                                         27
```

Fig. 5 - Example of a job deck composed of punched cards. Included are the control card deck, the "End of Records" and the data deck.

```
C2780,CM120000,P2. BARTELS                                    CARD 1
ACCOUNT,*****. ATABS                                            2
ATTACH,ATB,ATABSBIN,ID=JED,CY=10,MR=1.                          3
BEGIN,DISSPLA,,CAL1051,NAME=$BARTELS STOP 10$,                  4
TYPE=2,P1=NIB,S1=3,PAPER=11,XSIZE=100,B=ATB.                    5
*EOR                                                            6
PBCL2- 002          PBCL2 IN 0.1 N HCL                          7
<P>B<C>L2 BY <A A>$                                             8
<P>B<C>L2 (+M>G/G)$                                             9
<A>BSORBANCE$                                                  10
<P>B<C>L2- 002$                                                11
0.0 0.0                                                        12
5.0 0.185                                                      13
10.0 0.369                                                     14
20.0 0.649                                                     15
30.0 0.875                                                     16
*EOR                                                           17
0.396                                                          18
0.600                                                          19
0.455                                                          20
0.661                                                          21
0.460                                                          22
0.519                                                          23
0.325                                                          24
0.861                                                          25
*EOR                                                           26
*EOF                                                           27
```

**Fig. 6 - Example of a job deck in the form of a local file as it would be built in TXTEDIT or EDITOR and processed from an on-line terminal.**

```
**********  PLOT STATISTICS  **********

X-EXTENT=    10    Y-EXTENT=    11    (IN INCHES)
ESTIMATED PLOT TIME=   1.4 MINUTES
DSPACE USED=      19
APPROXIMATE PEN MOTION(INCHES)=      377.3
APPROXIMATE NO. OF VECTORS=       2928

PLOT WITH IDENTIFIER: C27805D19 FROM JOB: C278050    AT 19/02/82  09.59.02.


END OF DISSPLA 8.2 --      2926 VECTORS GENERATED IN      1 PLOT FRAMES.
-ISSCO-  4186 SORRENTO VALLEY BLVD.,SAN DIEGO CALIF. 92121

DISSPLA IS A CONFIDENTIAL PROPRIETARY PRODUCT OF ISSCO AND ITS USE
   IS SUBJECT TO A NONDISSEMINATION AND NONDISCLOSURE AGREEMENT.
```

**Fig. 7 - Plot statistics provided by DISSPLA**

```
  MFA  CSC CYBER 730 SN447 NOS/BE 1.4 L518 1352
09.57.42.C278050  FROM MFA/DC
09.57.42.IP  00001664 WORDS - FILE INPUT  , DC 04
09.57.42.C2780,CM120000,P2. BARTELS
09.57.43.SYSBULL(NO8UL)
09.57.43.FTN(R=3)
09.57.54.      1.881 CP SECONDS COMPILATION TIME
09.57.55.BEGIN,DISSPLA,,CAL105L,NAME=$BARTELS STO
09.57.55.P 10$,
09.57.56.AT CY= 165 SN=PUBLIC
09.57.57.TYPE=2,P1=NIB,SL=3,XSIZE=100.
09.57.59.IFE,$0$,NE.$0$,LGO.
09.58.00.ENDIF,LGO.
09.58.00.CASE(CAL105L)
09.58.00.SKIP,PLOTTER.
09.58.03.ENDIF,PLOTTER.
09.58.03.BEGIN,GETIT,,NUPLOTL.
09.58.04.IFE,,NOT.FILE(NUPLOTL,AS),NOTAT.
09.58.04.ATTACH,NUPLOTL,NUPLOTL,ID=PUBLIC,MR=1.
09.58.05.AT CY= 020 SN=PUBLIC
09.58.05.ENDIF,NOTAT.
09.58.05.REVERT.
09.58.05.REMARK. START OF PARAMETER CHECKING
09.58.05.LDSET(LIB=NUPLOTL).
09.58.06.GETPAR.CCRDEF,MF.
09.58.14.     STOP   PARAMETER CHECKING COMPLETED
09.58.14.RETURN,PF.
09.58.14.IFE,$PF$,EQ.$PF$,UDS.
09.58.15.MOUNT,VSN=EM2124,SN=PLOTTER.
09.58.16.MOUNTED VSN=EM2124,SN=PLOTTER
09.58.16.REQUEST,PF,*PF,SN=PLOTTER.
09.58.16.ELSE,UDS.
09.58.16.ENDIF,UDS.
09.58.16.BEGIN,RUNDIS,,CALCMPL,,$LGO$,$$,
09.58.16.PUBLIC,$0$,MAP=OFF,RFL=$0$.
09.58.17.BEGIN,GETIT,,CALCPPL,,PUBLIC.
09.58.18.IFE,,NOT.FILE(CALCPPL,AS),NOTAT.
09.58.19.ATTACH,CALCMPL,CALCMPL,ID=PUBLIC,MR=1.
09.58.19.AT CY= 020 SN=PUBLIC
09.58.19.ENDIF,NOTAT.
09.58.19.REVERT.
09.58.19.BEGIN,GETIT,,DISSPLA,$,SN=PUBLIC$,PUBLIC
09.58.19.,
09.58.21.IFE,,NOT.FILE(DISSPLA,AS),NOTAT.
09.58.21.ATTACH,DISSPLA,DISSPLA,SN=PUBLIC,ID=PUBL
09.58.21.IC,MR=1.
09.58.21.AT CY= 020 SN=PUBLIC
09.58.21.ENDIF,NOTAT.
09.58.21.REVERT.
09.58.22.BEGIN,GETIT,,DISPLA2,$,SN=PUBLIC$,PUBLIC
09.58.22.,
09.58.22.IFE,,NOT.FILE(DISPLA2,AS),NOTAT.
09.58.23.ATTACH,DISPLA2,DISPLA2,SN=PUBLIC,ID=PUBL
09.58.23.IC,MR=1.
09.58.23.AT CY= 020 SN=PUBLIC
09.58.23.ENDIF,NOTAT.
09.58.23.REVERT.
09.58.24.MAP,OFF.
09.58.24.IFE,$0$,EQ.$0$,DOIT.
09.58.24.LDSET(PRESET=ZERO)
09.58.24.LDSET(LIB=CALCMPL/DISSPLA/DISPLA2)
09.58.24.LGO.
09.58.51.( PF       ASSIGNED TO EST 025)
09.59.02.RETURN     HEADER
09.59.02.REQUEST(HEADER,*O,GY)
09.59.02.( HEADER: ASSIGNED TO EST 136)
09.59.02.OP  00000128 WORDS - FILE C278050, DC 30     *PLT  PT
09.59.03.CT ID=C274050J9 PFN=PF
09.59.03.CT CY= 001 SN=PLOTTER 0000001920 WORDS.
09.59.03.RETURN     PF
09.59.03.      END  ATABS
09.59.03.    104000 MAXIMUM EXECUTION FL.
09.59.03.      4.835 CP SECONDS EXECUTION TIME.
09.59.03.ENDIF,NORFL.
09.59.03.ELSE,DOIT.
09.59.03.ENDIF,DOIT.
09.59.03.MAP,OFF.
09.59.03.RETURN,CCRDEF.
09.59.04.REVERT.
09.59.04.RETURN,MF,CCRDEF,PF,HEADER.
09.59.04.REVERT.
09.59.04.OP  00004992 WORDS - FILE OUTPUT , DC 40
09.59.04.MAX STEP FL 0105008 ,MAX JOB FL 1200008
09.59.04.CPA      12.017 SEC.  (      148 SEC.): $        1.001
09.59.04.IO       59.222 SEC.  (      738 SEC.): $         .444
09.59.04.CM     2067.906 KWS.  (    40248 KWS.): $         .574
09.59.04.SS (P2 RATE/TAUX)                TOTAL: $        2.020
09.59.04.PP       98.319 SEC.     DATE 19/02/82
09.59.04.EJ  END OF JOB, DC
```

Fig. 8 - Complete job DAYFILE. Job name and plot

POOR

QUALITY

ORIGINAL